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VABILO NA PREDAVANJE
V OKVIRU DOKTORSKEGA ŠTUDIJA
KEMIJSKE ZNANOSTI

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z naslovom:

Virus self-assembly modeling

v sredo, 11. marca 2015 ob 15:00 uri
v predavalnici 1 v 1. nadstropju Fakultete
za kemijo in kemijsko tehnologijo, Večna pot 113

Vljudno vabljeni!

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Abstract

The structural organization of viruses is characterized by simplicity and economy. At a minimal level, the viral genome is composed of either single or double stranded RNA or DNA, surrounded by a spherical-like or cylindrical protein shell composed of many copies of almost identical proteins. The linear size of the virus genome can be tens of microns and is large compared to the diameter of capsid, usually in the range of tens of nanometers, so the genome must undergo a high degree of compaction during viral assembly. *In vivo*, (1) spherical-like viruses with double-stranded genome are made in two steps; first an empty capsid is formed and thereafter the genome is actively transferred into the capsid, whereas (2) spherical-like viruses with single-stranded genome are formed by a co-assembly of capsid subunits and the genome.

During the last decade, spherical-like viruses have been subjected to theoretical modeling using descriptions of different degree of details. Here, results from molecular dynamic studies of a coarse-grain model describing the process of forming single-stranded viruses possessing icosahedral symmetry will be discussed. The assembly process was investigated for capsomers with different net charge and charge distribution in combination with linear, branched, and hyper-branched polyions, and characterized in terms of the time-dependent cluster size probabilities, averaged cluster size, encapsulation efficiency, and polyion extension.